09/868,944

- Active
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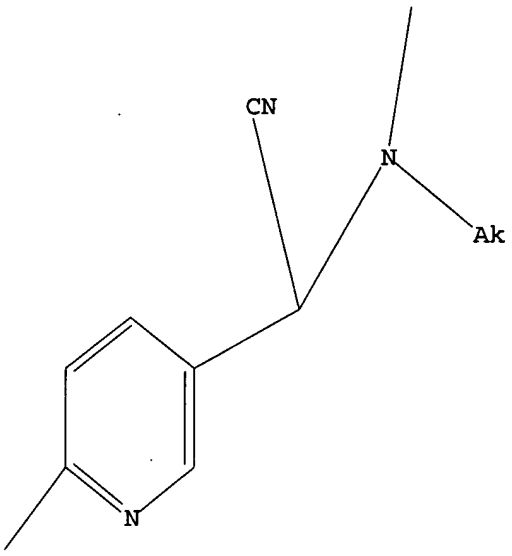
  - L2: (1086705) pyridyl(w)acetonitril
  - L3: (1117702) pyridyl(w)acetonitrile
  - L4: (107116) pyridyl(1w)acetonitrile
  - L5: (127063) pyridyl(w1)acetonitrile
  - L6: (463) l4 and (546/?).ccls.
  - L7: (16) l6 and vinylpyridine

09/868,944

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful
FULL SEARCH INITIATED 15:41:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 72 TO ITERATE

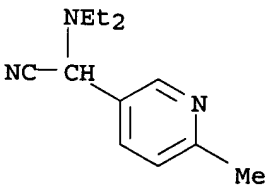
100.0% PROCESSED 72 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

L2 1 SEA SSS FUL L1

=>

=> d

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
RN 283167-57-7 REGISTRY
ED Entered STN: 04 Aug 2000
CN 3-Pyridineacetonitrile, α-(diethylamino)-6-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H17 N3
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	163.17	163.38

FILE 'CAPLUS' ENTERED AT 15:41:36 ON 10 NOV 2005
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FILE COVERS 1907 - 10 Nov 2005 VOL 143 ISS 20
FILE LAST UPDATED: 9 Nov 2005 (20051109/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l2
L3 1 L2

=> d fbib abs fhitstr

L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:493518 CAPLUS
DN 133:104966
TI Preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone.
IN Armbruster, Erich; Bessard, Yves; Kuo, David; Leresche, James Edward; Proplesch, Ralf; Roduit, Jean-Paul
PA Lonza A.-G., Switz.; Merck & Co., Inc.
SO PCT Int. Appl., 19 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000042014	A2	20000720	WO 2000-EP240	20000113
	WO 2000042014	A3	20001207		

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

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				US 1999-145996P	P	19990729
				WO 2000-EP240	W	20000113
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				US 1999-145996P	P	19990729
				CA 2000-2359958	A3	20000113
EP 1159270		A2	20011205	EP 2000-901555		20000113
EP 1159270		B1	20031105			

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JP 2003518002		T2	20030603	JP 2000-593582		20000113
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				US 1999-145996P	P	19990729
				WO 2000-EP240	W	20000113
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				WO 2000-EP240	W	20000113
EP 1394149		A1	20040303	EP 2003-24787		20000113
EP 1394149		B1	20050119			

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY

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ES 2209807		T3	20040701	ES 2000-901555		20000113
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				US 1999-145996P	P	19990729
AT 287396		E	20050215	AT 2003-24787		20000113
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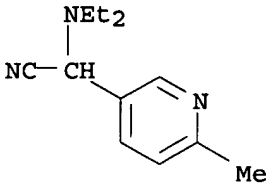
PT 1394149		T	20050531	PT 2003-24787		20000113
				EP 1999-100590	A	19990114
ES 2235138		T3	20050701	ES 2003-3024787		20000113
				EP 1999-100590	A	19990114
				WO 2000-EP240	W	20000113
NO 2001003498		A	20010905	NO 2001-3498		20010713
				EP 1999-100590	A	19990114
				US 1999-145996P	P	19990729
				WO 2000-EP240	W	20000113
US 2005159458		A1	20050721	US 2005-29489		20050106
				EP 1999-100590	A	19990114
				US 1999-145996P	P	19990729
				WO 2000-EP240	W	20000113
				US 2003-868941	A3	20031104

OS CASREACT 133:104966

AB 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone (I), useful as a starting material for cyclooxygenase-2 inhibitors, was prepared Thus, N,N-diethyamino(6-methylpyridin-3-yl)acetonitrile (preparation given) and celite in PhMe were treated sequentially with aqueous NaOH, tetrabutylammonium bromide, a solution of tetrabutylammonium bromide and 4-methylsulfonylbenzyl bromide in PhMe, and tetrabutylammonium bromide followed by stirring for 6 h at 45° to give 76.4% I.

IT **283167-57-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone)
RN 283167-57-7 CAPLUS
CN 3-Pyridineacetonitrile, α-(diethylamino)-6-methyl- (9CI) (CA INDEX NAME)



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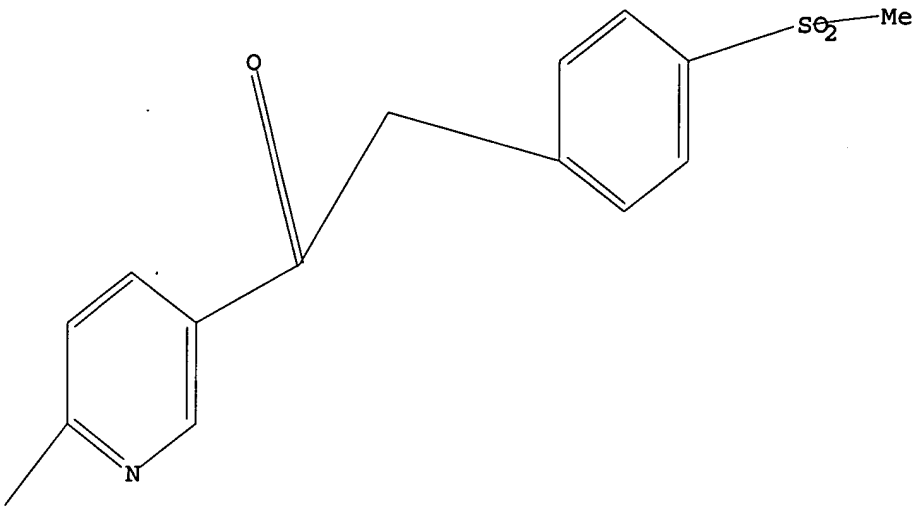

Structure attributes must be viewed using STN Express query preparation.

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=> s l4 ful
FULL SEARCH INITIATED 15:43:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       20 TO ITERATE

100.0% PROCESSED       20 ITERATIONS                                  4 ANSWERS
SEARCH TIME: 00.00.01

L5            4 SEA SSS FUL L4

=> d 1-4

L5   ANSWER 1 OF 4  REGISTRY  COPYRIGHT 2005 ACS on STN
RN   788151-35-9  REGISTRY
ED   Entered STN:  25 Nov 2004
CN   Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]-, ion(1-)
     (9CI)  (CA INDEX NAME)
FS   3D CONCORD
MF   C15 H14 N O3 S
CI   COM
SR   CA
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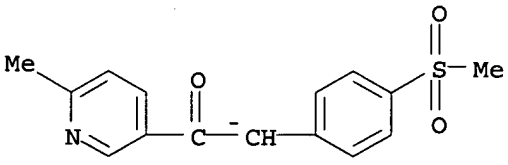


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L5   ANSWER 2 OF 4  REGISTRY  COPYRIGHT 2005 ACS on STN
RN   452332-13-7  REGISTRY
ED   Entered STN:  18 Sep 2002
CN   1-Propanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
     (CA INDEX NAME)
FS   3D CONCORD
MF   C16 H17 N O3 S
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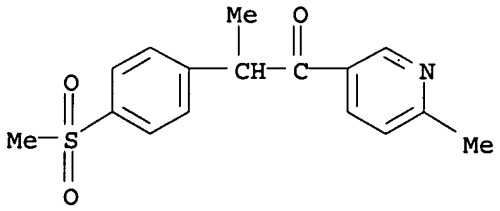
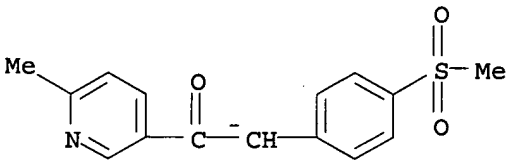
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

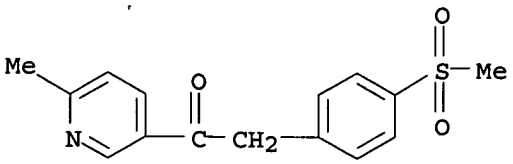
L5 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
RN 452332-12-6 REGISTRY
ED Entered STN: 18 Sep 2002
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]-, ion(1-), potassium (9CI) (CA INDEX NAME)
MF C15 H14 N O3 S . K
SR CA
LC STN Files: CA, CAPLUS
CRN (788151-35-9)



● K^+

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
RN 221615-75-4 REGISTRY
ED Entered STN: 25 Apr 1999
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
FS 3D CONCORD
MF C15 H15 N O3 S
SR CA
LC STN Files: BIOSIS, CA, CAPLUS, CASREACT, PS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

16 REFERENCES IN FILE CA (1907 TO DATE)
16 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	168.69	338.36

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.73

FILE 'CAPLUS' ENTERED AT 15:43:52 ON 10 NOV 2005
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FILE COVERS 1907 - 10 Nov 2005 VOL 143 ISS 20
FILE LAST UPDATED: 9 Nov 2005 (20051109/ED)

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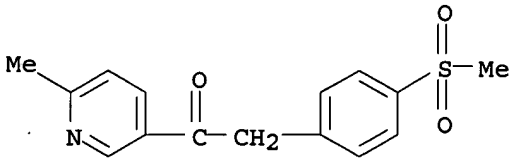
http://www.cas.org/infopolicy.html

=> s l5
L6 16 L5

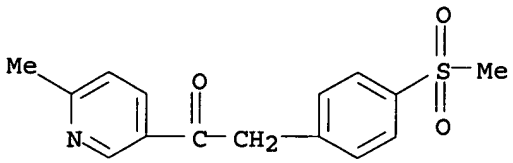
=> d 1-16 fbib abs fhitstr

L6 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2005:406839 CAPLUS
Correction of: 2005:155216
DN 143:248209
Correction of: 142:197768
TI Product class 1: pyridines
AU Spitzner, D.
CS Germany
SO Science of Synthesis (2005), 15, 11-284
CODEN: SSCYJ9
PB Georg Thieme Verlag

DT Journal; General Review
LA English
AB A review of methods to prepare pyridines, pyridine-1-oxides, and pyridinium salts. Methods include cyclization, ring transformations, aromatization and substituent modification.
IT **221615-75-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(review of preparation of pyridines, pyridine-1-oxides and pyridinium salts via cyclization, ring transformations, aromatization and substituent modification)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



L6 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:586395 CAPLUS
DN 140:117549
TI Development and validation of an HPLC method for the impurity and quantitative analysis of etoricoxib
AU Hartman, Robert; Abrahim, Ahmed; Clausen, Andrew; Mao, Bing; Crocker, Louis S.; Ge, Zhihong
CS Analytical Research, Merck Research Laboratories, Rahway, NJ, 07065-0914, USA
SO Journal of Liquid Chromatography & Related Technologies (2003), 26(15), 2551-2566
CODEN: JLCTFC; ISSN: 1082-6076
PB Marcel Dekker, Inc.
DT Journal
LA English
AB Etoricoxib (5-chloro-6'-methyl-3[4-(methanesulfonyl)phenyl]-2,3'-bipyridine) is a highly active and selective cyclo-oxygenase II inhibitor. A single, stability-indicating HPLC method was developed and validated for both the impurity and quant. anal. of etoricoxib. Method development incorporated the optimization of stationary phase, pH, temperature, and mobile phase composition for the resolution of 13 process impurities and 3 major degradation products. Further optimization of pH and mobile phase composition was aided by the use of DryLab, a computer-based simulation program. The stability-indicating capability of the method was proven through the identification of photolytic and oxidative decomposition products. Method validation produced excellent results for linearity, precision, limit of quantitation and limit of detection, specificity, accuracy, recovery, and robustness. The identities of etoricoxib decomposition products were confirmed by UV, LC/MS, and NMR spectra.
IT **221615-75-4**
RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)
(development and validation of an HPLC method for the impurity and quant. anal. of etoricoxib)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

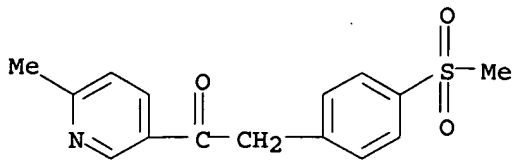


RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:491189 CAPLUS
DN 139:70705
TI Production of methylpyridinyl methylsulfonylphenyl ethanone by oxidation of the respective methylthiophenyl derivative
IN Cannata, Vincenzo; Soriato, Giorgio; Verzini, Massimo
PA Zambon Group S.P.A., Italy
SO PCT Int. Appl., 10 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

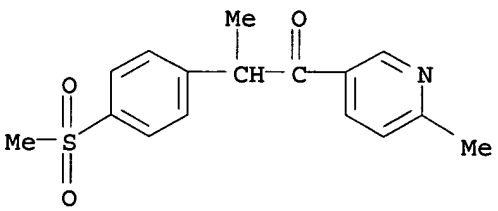
	PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
PI	WO 2003051843	A1	20030626	WO 2002-EP14115		20021212
	W: CN, CZ, HU, IL, IN, US					
	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR					
				IT 2001-MI2692	A	20011219
	EP 1492770	A1	20050105	EP 2002-795165		20021212
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, CY, TR, BG, CZ, EE, SK					
				IT 2001-MI2692	A	20011219
				WO 2002-EP14115	W	20021212
	US 2005165238	A1	20050728	US 2003-499321		20021212
				IT 2001-MI2692	A	20011219
				WO 2002-EP14115	W	20021212

OS CASREACT 139:70705
AB A process for production of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone is carried out by oxidation of 1-(6-methylpyridin-3-yl)-2-[4-(methylthio)phenyl]ethanone with an oxidant in the presence of an acid, the oxidant being a mixture of peracetic acid and hydrogen peroxide, and the acid being methanesulfonic acid. The product is useful as an intermediate in production of cyclooxygenase 2 (COX 2) inhibitors. Thus, the title compound was produced in 88.6% yield by mixing 1-(6-methylpyridin-3-yl)-2-[4-(methylthio)phenyl]ethanone (30), acetic acid (45), methanesulfonic acid (13.6), adding Oxystrong (65% peracetic acid) (28.1 kg) at 35°, and reacting the mixture at 35° for 3-4 h.
IT **221615-75-4P**, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
RL: IMF (Industrial manufacture); PREP (Preparation)
(production of methylpyridinyl methylsulfonylphenyl ethanone by oxidation of resp. methylthiophenyl derivative)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:434902 CAPLUS
DN 137:210102
TI Development of a derivatization method, coupled with reverse phase HPLC, for monitoring the formation of an enolate intermediate
AU Abrahim, A.; Hartman, R.; Ge, Z.; Mao, B.; Marcoux, J.
CS Merck Research Laboratories, Rahway, NJ, 07065-0914, USA
SO Journal of Liquid Chromatography & Related Technologies (2002), 25(7), 1049-1062
CODEN: JLCTFC; ISSN: 1082-6076
PB Marcel Dekker, Inc.
DT Journal
LA English
AB A sensitive liquid chromatog. method was developed to monitor the formation of an enolate intermediate in a synthetic route to Etoricoxib, a drug candidate for the treatment of arthritis. The method requires the derivatization of the enolate with Me iodide to form a stable methylketosulfone derivative followed by reverse phase HPLC anal. Parameters affecting the derivatization, including the nature of derivatizing agent, reaction solvent, amount of derivatizing agent, reaction time, reaction temperature, and amount of excess base in the reaction were studied. The derivatization reaction gave selective C-alkylation. The linear range of the chromatog. method for the determination of the starting material, ketosulfone, and the derivative, methylketosulfone, was determined Finally, the accuracy of the method was established based on recovery expts.
IT **452332-13-7**
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(LC-mass spectra of)
RN 452332-13-7 CAPLUS
CN 1-Propanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



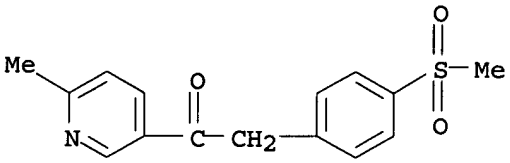
RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:276519 CAPLUS
DN 136:310188
TI Treatment of cancer with a prostate specific antigen (PSA) conjugate and an NSAID compound

IN Heimbrook, David C.; Yao, Siu-long
PA USA
SO U.S. Pat. Appl. Publ., 129 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
PI US 2002042375	A1	20020411	US 2001-896245		20010629
			US 2000-216217P	P	20000705

OS MARPAT 136:310188
AB The invention relates to methods of treating cancer using a combination of a compound which is a PSA conjugate and a nonsteroidal antiinflammatory agent (NSAID) and to methods of preparing such compns. The PSA conjugate comprises an oligopeptide that is selectively cleaved by PSA and a cytotoxic agent. An example of a PSA conjugate is N-Ac-(4-trans-L-Hyp)-Ala-Ser-Chg-Gln-Ser-Leu-Dox (Dox = doxorubicin, Hyp = hydroxyproline, Chg = cyclohexylglycine) and COX-2 inhibitor 3-phenyl-4-[4-(4-methylsulfonyl)phenyl]-2(5H)furanone is an example of an NSAID compound (syntheses given).
IT **221615-75-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(treatment of cancer with prostate specific antigen (PSA) conjugate and NSAID compound)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



L6 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:886073 CAPLUS
DN 136:11103
TI 5-chloro-3-(4-methanesulfonylphenyl)-6'-methyl- [2,3']bipyridinyl in pure crystalline form and process for synthesis
IN Crocker, Louis S.; Davies, Ian W.; Osifchin, Richard G.; Kotliar, Andrew
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001092230	A1	20011206	WO 2001-US16566	20010522

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

				US 2000-208017P	P	20000526
	CA 2410234	AA	20011206	CA 2001-2410234		20010522
				US 2000-208017P	P	20000526
				WO 2001-US16566	W	20010522
	EP 1296951	A1	20030402	EP 2001-939267		20010522
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
				US 2000-208017P	P	20000526
				WO 2001-US16566	W	20010522
	JP 2004501116	T2	20040115	JP 2002-500844		20010522
	JP 3665053	B2	20050629			
				US 2000-208017P	P	20000526
				WO 2001-US16566	W	20010522
	NZ 522394	A	20040528	NZ 2001-522394		20010522
				US 2000-208017P	P	20000526
				WO 2001-US16566	W	20010522
	EE 200200655	A	20040816	EE 2002-655		20010522
				US 2000-208017P	P	20000526
				WO 2001-US16566	W	20010522
	BR 2001011140	A	20050111	BR 2001-11140		20010522
				US 2000-208017P	P	20000526
				WO 2001-US16566	W	20010522
	BG 107237	A	20030530	BG 2002-107237		20021031
				US 2000-208017P	P	20000526
				WO 2001-US16566	W	20010522
	ZA 2002009558	A	20031028	ZA 2002-9558		20021125
				US 2000-208017P	P	20000526
	JP 2005047927	A2	20050224	JP 2004-263913		20040910
				US 2000-208017P	P	20000526
				JP 2002-500844	A3	20010522

PATENT FAMILY INFORMATION:

FAN 2002:778724

	PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
PI	US 2002147221	A1	20021010	US 2001-957966		20010921
	US 6800647	B2	20041005			
				US 2000-208017P	P	20000526
				US 2001-865771	A2	20010525
	US 2002016343	A1	20020207	US 2001-865771		20010525
	US 6521642	B2	20030218			
				US 2000-208017P	P	20000526
	CA 2447878	AA	20021205	CA 2001-2447878		20010921
				US 2001-865771	A	20010525
				WO 2001-US29551	W	20010921
	WO 2002096877	A1	20021205	WO 2001-US29551		20010921
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
				US 2001-865771	A	20010525
	EP 1395562	A1	20040310	EP 2001-973314		20010921
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
				US 2001-865771	A	20010525
				WO 2001-US29551	W	20010921
	JP 2004530706	T2	20041007	JP 2003-500057		20010921
				US 2001-865771	A	20010525
				WO 2001-US29551	W	20010921
	US 2003153600	A1	20030814	US 2003-342380		20030114

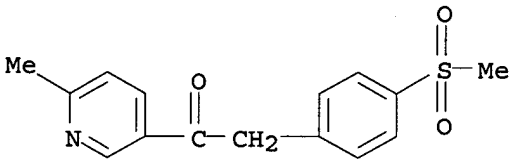
US 6673935	B2	20040106			
			US 2001-865771	A3	20010525
JP 2005047927	A2	20050224	JP 2004-263913		20040910
			US 2000-208017P	P	20000526
			JP 2002-500844	A3	20010522

AB This invention encompasses the form V polymorph of the title composition which is useful in the treatment of cyclooxygenase-2 mediated diseases. The invention encompasses certain pharmaceutical compns. for treatment of cyclooxygenase-2 mediated diseases comprising the Form V polymorph of the title composition The invention also encompasses a process for synthesizing the form V polymorph of the title composition A mixture of the title composition and
iso-Pr acetate was heated at 55°, then was cooled to ambient temperature and the solids were isolated by filtration. The solids were washed with iso-Pr acetate and dried in vacuo to give the form V polymorph as a colorless solid in about 87% yield.

IT **221615-75-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(methanesulfonylphenylmethyl bipyridinyl in pure crystalline form and process for synthesis)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:300685 CAPLUS
DN 134:311114
TI Process for the oxidation of 1-(6-methyl-3-pyridinyl)-2-[4-(methylthio)phenyl]ethanone into 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone
IN Cannata, Vincenzo; Rossato, Roberto
PA Zambon Group S.P.A., Italy
SO PCT Int. Appl., 9 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001029004	A1	20010426	WO 2000-EP9995	20001011
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
			IT 1999-MI2156	A 19991015
IT 99MI2156	A1	20010416	IT 1999-MI2156	19991015

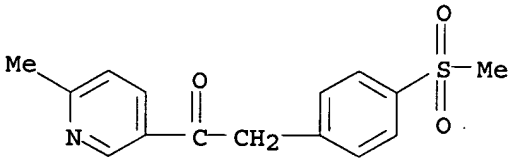
OS CASREACT 134:311114

AB A process for the oxidation of 1-(6-methyl-3-pyridinyl)-2-[4-(methylthio)phenyl]ethanone (I) into 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone, a pharmaceutical intermediate (no data), without the formation of N-oxide byproduct, consists of reacting I with an oxidant (e.g., a mixture of peracetic acid and hydrogen peroxide) in the presence of a catalyst (e.g., sodium tungstate) and an acid (e.g. methanesulfonic acid).

IT **221615-75-4P**, 1-(6-Methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for the oxidation of 1-(6-methyl-3-pyridinyl)-2-[4-(methylthio)phenyl]ethanone into 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:300684 CAPLUS

DN 134:295751

TI Process for the preparation of intermediates useful in the synthesis of diarylpyridines

IN Allegrini, Pietro; Verzini, Massimo

PA Zambon Group S.P.A., Italy

SO PCT Int. Appl., 20 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001029003	A1	20010426	WO 2000-EP9994	20001011
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
			IT 1999-MI2157	A 19991015
IT 99MI2157	A1	20010416	IT 1999-MI2157	19991015

OS CASREACT 134:295751; MARPAT 134:295751

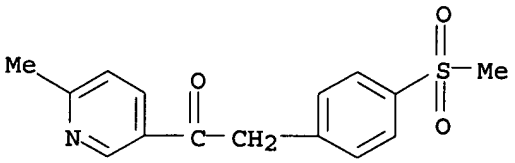
AB This process is used to prepare intermediates useful in the synthesis of diarylpyridines having COX-2 inhibitor activity. E.g., reaction of 6-methylnicotinic acid Me ester with (4-methylthiophenyl)acetonitrile gave 3-(6-methylpyridin-3-yl)-2-(4-methylthiophenyl)-3-oxopropionitrile hydrochloride. Acid hydrolysis and decarboxylation of the latter gave 1-(6-methylpyridin-3-yl)-2-(4-methylthiophenyl)ethanone.

IT **221615-75-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)

(process for the preparation of intermediates useful in the synthesis of diarylpyridines)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:185752 CAPLUS

DN 134:222716

TI 1,2,3-Thiadiazoles and their use as COX-2 inhibitors

IN Lau, Cheuk K.; Li, Chun Sing; Therien, Michel; Gauthier, Jacques Y.

PA Merck Frosst Canada & Co., Can.

SO PCT Int. Appl., 45 pp.
CODEN: PIXXD2

DT Patent

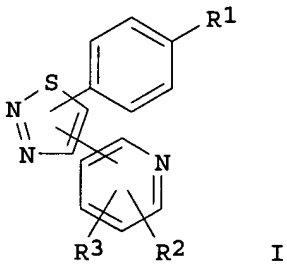
LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001017996	A1	20010315	WO 2000-CA1040	20000907
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
			US 1999-152746P	P 19990908

OS MARPAT 134:222716

GI



I

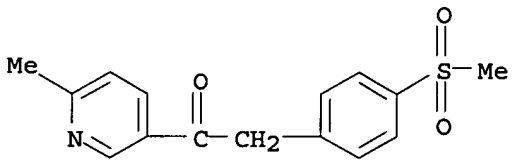
AB Title compds. I [R1 = SO2Me, S(O)NHMe, S(O)NHNH2, P(O)MeOH, etc.; R2, R3 = H, halo, alkoxy, alkyl, CN, etc.] were prepared Thus, 4-(6-methyl-3-pyridinyl)-5-[4-(methylsulfonyl)phenyl]-1,2,3-thiadiazole (II) was prepared in 5 steps starting from 6-methylnicotinic acid and N-methoxymethylamine hydrochloride. Oxidation of II with H2O2 gave the thiadiazole 3-oxide.

Inhibition of COX-2 was determined by measuring the effects on PGE2 production in whole blood.

IT **221615-75-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(1,2,3-thiadiazoles as COX-2 inhibitors)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:78362 CAPLUS
DN 134:131435
TI Preparation of 1-(6-methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl]ethanone starting from 4-methylthiobenzyl alcohol and 6-methylnicotinate esters.
IN Bessard, Yves; Leresche, James Edward
PA Lonza A.-G., Switz.; Merck & Co., Inc.
SO PCT Int. Appl., 15 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001007410	A1	20010201	WO 2000-EP6825	20000717
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
			EP 1999-114667	A 19990727
			US 2000-186680P	P 20000303
EP 1198455	A1	20020424	EP 2000-951393	20000717
EP 1198455	B1	20031210		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, MC, IE, SI, LT, LV, FI, RO, MK, CY, AL				
			EP 1999-114667	A 19990727
			US 2000-186680P	P 20000303
			WO 2000-EP6825	W 20000717
JP 2003505449	T2	20030212	JP 2001-512497	20000717
			EP 1999-114667	A 19990727
			US 2000-186680P	P 20000303
			WO 2000-EP6825	W 20000717
AT 256112	E	20031215	AT 2000-951393	20000717
			EP 1999-114667	A 19990727
			US 2000-186680P	P 20000303

			WO 2000-EP6825	W	20000717
ES 2207536	T3	20040601	ES 2000-951393		20000717
			EP 1999-114667	A	19990727
			US 2000-186680P	P	20000303
US 6566527	B1	20030520	US 2002-30096		20020314
			EP 1999-114667	A	19990727
			US 2000-186680P	P	20000303
			WO 2000-EP6825	W	20000717
US 2003088107	A1	20030508	US 2002-283167		20021030
US 6600046	B2	20030729			
			EP 1999-114667	A	19990727
			US 2000-186680P	P	20000303
			WO 2000-EP6825	W	20000717
			US 2002-30096	A3	20020314

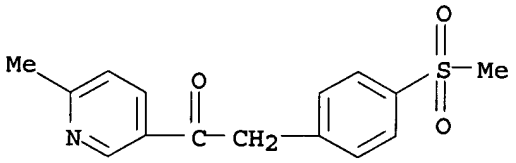
OS CASREACT 134:131435

AB 1-(6-Methylpyridin-3-yl)-2-[(4-methylsulfonyl)phenyl]ethanone was prepared by (a) treatment of 4-(methylthio)benzyl alc. with hydrochloric acid to give 4-(methylthio)benzyl chloride, (b) treatment of this with an alkali metal cyanide to give 4-(methylthio)phenylacetonitrile, (c) condensation of 4-(methylthio)phenylacetonitrile with a 6-methylnicotinate ester to give 3-[2-(4-methylthiophenyl)-2-cyanoacetyl]-6-methylpyridine, (d) hydrolysis and decarboxylation under acidic conditions to give 3-[2-(4-methylthiophenyl)acetyl]-6-methylpyridine and (e) oxidation

IT **221615-75-4P**, 1-(6-Methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl]ethanone
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of 1-(6-methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl]ethanone starting from 4-methylthiobenzyl alc. and 6-methylnicotinate esters)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:897114 CAPLUS

DN 134:178439

TI A general [3 + 2 + 1] annulation strategy for the preparation of pyridine N-oxides

AU Davies, Ian W.; Marcoux, Jean-Francois; Reider, Paul J.

CS Department of Process Research, Merck & Co. Inc., Rahway, NJ, 07065, USA

SO Organic Letters (2001), 3(2), 209-211
CODEN: ORLEF7; ISSN: 1523-7060

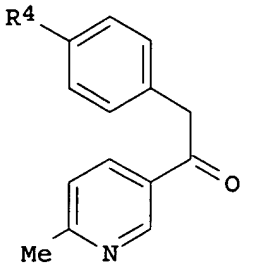
PB American Chemical Society

DT Journal

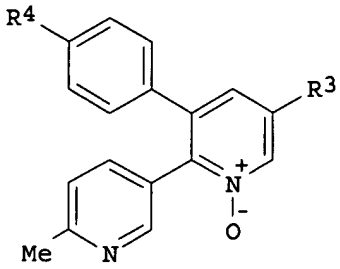
LA English

OS CASREACT 134:178439

GI



I



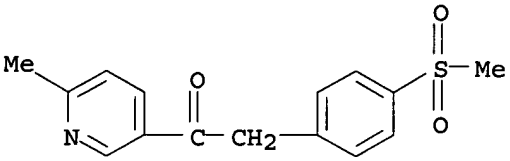
II

AB Stabilized ketone, aldehyde, and ester enolates, generated from I (R4 = MeSO2, MeS) for example, react with vinamidinium hexafluorophosphate salts and hydroxylamine hydrochloride to give pyridine N-oxides, e.g. II (R3 = Cl, NO2), in 45-85% yields.

IT **221615-75-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyridine N-oxides by cyclization of vinamidinium salts with enolates of ketones, aldehydes, and esters)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:653182 CAPLUS

DN 134:4838

TI A Practical Synthesis of a COX-2-Specific Inhibitor

AU Davies, Ian W.; Marcoux, Jean-Francois; Corley, Edward G.; Journet, Michel; Cai, Dong-Wei; Palucki, Michael; Wu, Jimmy; Larsen, Robert D.; Rossen, Kai; Pye, Philip J.; DiMichele, Lisa; Dormer, Peter; Reider, Paul J.

CS Department of Process Research, Merck Co. Inc., Rahway, NJ, 07065, USA

SO Journal of Organic Chemistry (2000), 65(25), 8415-8420
CODEN: JOCEAH; ISSN: 0022-3263

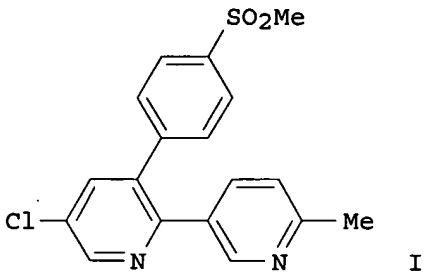
PB American Chemical Society

DT Journal

LA English

OS CASREACT 134:4838

GI



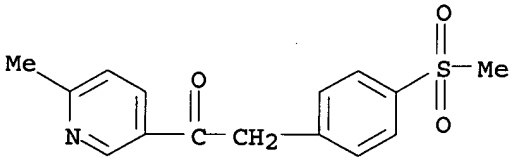
I

AB A number of synthetic strategies to the Cox-2 specific inhibitor have been described. These studies have led to the identification of a novel pyridine construction using annulation of a ketone using a vinamidinium species and ammonia in 97% assay yield. Three approaches to the synthesis of the ketone are described that allow for its preparation in large quantities in >65% overall yield from Me 6-methylnicotinate.

IT **221615-75-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of a methylsulfonylphenylbipyridine COX-2 inhibitor)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:493518 CAPLUS

DN 133:104966

TI Preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone.

IN Armbruster, Erich; Bessard, Yves; Kuo, David; Leresche, James Edward; Proplesch, Ralf; Roduit, Jean-Paul

PA Lonza A.-G., Switz.; Merck & Co., Inc.

SO PCT Int. Appl., 19 pp.
CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2000042014	A2	20000720	WO 2000-EP240	20000113
WO 2000042014	A3	20001207		

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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,

CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

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			US 1999-145996P	P	19990729
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			EP 1999-100590	A	19990114
			US 1999-145996P	P	19990729
			WO 2000-EP240	W	20000113
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			EP 1999-100590	A	19990114
			US 1999-145996P	P	19990729
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EP 1159270	A2	20011205	EP 2000-901555		20000113
EP 1159270	B1	20031105			

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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY

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			WO 2000-EP240	W	20000113
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			WO 2000-EP240	W	20000113
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			WO 2000-EP240	W	20000113
			US 2003-868941	A3	20031104

OS CASREACT 133:104966

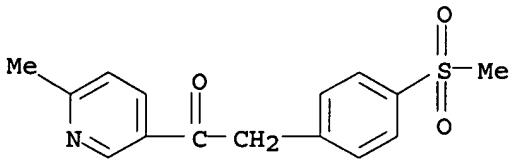
AB 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone (I), useful as a starting material for cyclooxygenase-2 inhibitors, was prepared Thus, N,N-diethyamino(6-methylpyridin-3-yl)acetonitrile (preparation given) and celite in PhMe were treated sequentially with aqueous NaOH, tetrabutylammonium bromide, a solution of tetrabutylammonium bromide and 4-methylsulfonylbenzyl bromide in PhMe, and tetrabutylammonium bromide followed by stirring for 6 h at 45° to give 76.4% I.

IT **221615-75-4P**, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



L6 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:443023 CAPLUS

DN 133:222553

TI Annulation of Ketones with Vinamidinium Hexafluorophosphate Salts: An Efficient Preparation of Trisubstituted Pyridines

AU Marcoux, Jean-Francois; Corley, Edward G.; Rossen, Kai; Pye, Phil; Wu, Jimmy; Robbins, Michael A.; Davies, Ian W.; Larsen, Robert D.; Reider, Paul J.

CS Department of Process Research, Merck Co. Inc., Rahway, NJ, 07065, USA

SO Organic Letters (2000), 2(15), 2339-2341
CODEN: ORLEF7; ISSN: 1523-7060

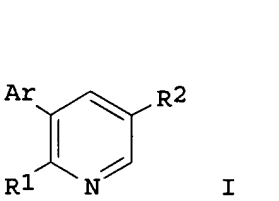
PB American Chemical Society

DT Journal

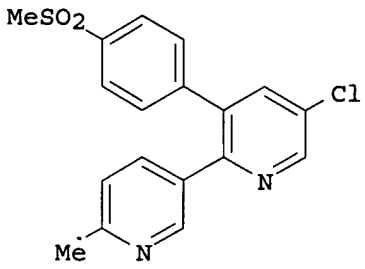
LA English

OS CASREACT 133:222553

GI



I



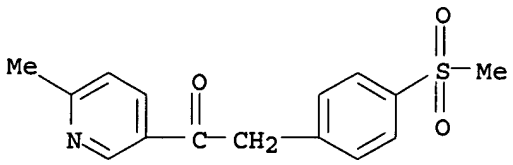
II

AB α-Aryl ketones react with vinamidinium hexafluorophosphate salts to give access to the corresponding 3-arylpyridines I (Ar = C6H4R-4, R = SO2Me, H, SMe, R1 = 6-methyl-3-pyridyl, C6H4R-4, R2 = Cl; Ar = C6H4SO2Me-4, R1 = 6-methyl-3-pyridyl, R2 = Br, I, CF3, NO2, phthalimido; Ar = C6H4F-4, R1 = Me, R2 = Cl; Ar = Ph, R1 = H, R2 = Cl). The annulation reactions proceed in good to excellent yields with vinamidinium salts containing electron-withdrawing groups at the β-position (R2). The reaction was applied to the preparation of the COX-2 specific inhibitor 5-chloro-3-(4-methylsulfonyl)phenyl-2-(2-methyl-5-pyridinyl)pyridine (II), as well as a series of analogs.

IT **221615-75-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of trisubstituted pyridines via annulation of ketones with vinamidinium hexafluorophosphate salts)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:708874 CAPLUS
DN 131:322542
TI Process for synthesizing arylpyridine COX-2 inhibitors
IN Corley, Edward G.; Davies, Ian W.; Larsen, Robert D.; Pye, Philip J.; Rossen, Kai
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 29 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
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PT 1071745	T	20041130	PT 1999-918706		19990420
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HK 1031399	A1	20041217	HK 2001-102195		20010326
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			US 1998-85668P	P	19980515
			WO 1999-US8645	A	19990420

OS CASREACT 131:322542; MARPAT 131:322542

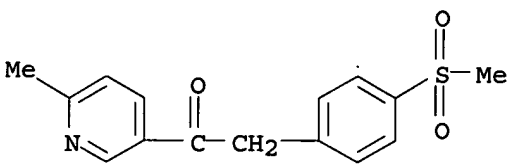
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention encompasses a process and intermediates for preparing compds. I [R, R', R'' = (un)substituted alkyl, aryl, aralkyl, halo, SOmH, SOm-alkyl, SOm-aryl, NO2, (di)(alkyl)amino, SOmNH2, SOmNH-alkyl, SOmNHCOCF3, cyano; Y = C, N; m = 0, 1, 2]. I are useful in the treatment of cyclooxygenase-2 mediated diseases (no data), i.e., as analgesics, antipyretics, and antiinflammatories. The method comprises cyclocondensation of an iminium salt II [R2-R5 = alkyl, aryl, or aralkyl; X- = suitable counterion] with an aryl ketone III in the presence of a base. The method is designed to give high yields at low temps., and with a reduced number of steps. For instance, the bipyridyl derivative IV was prepared on a 1.65-kg scale by reaction of the iminium salt V with ketone VI in THF in the presence of KOBu-tert, followed by quenching in AcOH/THF, basification with concentrated aqueous NH4OH, and refluxing. Prepns. of the salt and ketone intermediates V and VI are described, and a subset of the iminium salt intermediates II are claimed per se.

IT **221615-75-4P**, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of arylpyridine COX-2 inhibitors by cyclocondensation of iminium salts with ketones)

RN .221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



L6 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:222917 CAPLUS
DN 130:252250
TI Preparation of 3-phenyl-2-(3-pyridyl)pyridines and intermediates.
IN Davies, Ian W.; Gerena, Linda; Journet, Michel; Larsen, Robert D.; Pye, Philip J.; Rossen, Kai
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

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			GB 1998-6419	A	19980325
			WO 1998-US19788	W	19980922

OS CASREACT 130:252250; MARPAT 130:252250

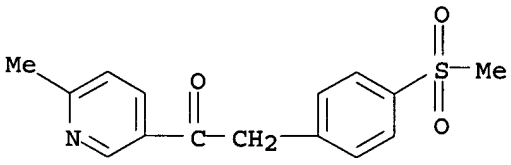
AB P-(ArCOCH2)C6H4SO2R1 (R1 = Me, NH2, NHCOCF3, NHMe; Ar = mono-, di-, or trisubstituted Ph, pyridyl, N-oxide thereof), were prepared by reaction of p-MeSC6H4CH2MgX (X = Cl, Br, F, iodo) with ArCONMe2 (Ar as above) to give p-(ArCOCH2)C6H4SMe followed by oxidation of the latter. Thus, the Grignard reagent from p-MeSC6H4CH2Cl in PhMe/THF was added to a -20° solution of 6-methylnicotinic acid N-methyl-N-methoxyamide (preparation given) in PhMe over 30 min. followed by 1 h aging to give 76% 2-methyl-5-(4-methylthiophenylacetyl)pyridine. The latter in MeOH/H2SO4 at 55° was treated with aqueous Na tungstate and then with H2O2 over 1 h to give 82.5% 2-methyl-5-(4-methylsulfonylphenylacetyl)pyridine. The latter reacted with 3-amino-2-chloroacrolein (preparation given) to give 65% 5-chloro-2-(2-methylpyrid-5-yl)-3-(4-methylsulfonylphenyl)pyridine.

IT **221615-75-4P**

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-phenyl-2-(3-pyridyl)pyridines and intermediates)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



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L3   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2005 ACS on STN
AN   2000:493518  CAPLUS
DN   133:104966
TI   Preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethano
     ne.
IN   Armbruster, Erich; Bessard, Yves; Kuo, David; Leresche, James Edward;
     Proplesch, Ralf; Roduit, Jean-Paul
PA   Lonza A.-G., Switz.; Merck & Co., Inc.
SO   PCT Int. Appl., 19 pp.
     CODEN: PIXXD2
DT   Patent
LA   German
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.         DATE
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PI   WO 2000042014        A2    20000720    WO 2000-EP240           20000113
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             IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
             MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
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             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
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			US 2003-868941	A3	20031104

OS CASREACT 133:104966

AB 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone (I), useful as a starting material for cyclooxygenase-2 inhibitors, was prepared Thus, N,N-diethyamino(6-methylpyridin-3-yl)acetonitrile (preparation given) and celite in PhMe were treated sequentially with aqueous NaOH, tetrabutylammonium bromide, a solution of tetrabutylammonium bromide and 4-methylsulfonylbenzyl bromide in PhMe, and tetrabutylammonium bromide followed by stirring for 6 h at 45° to give 76.4% I.

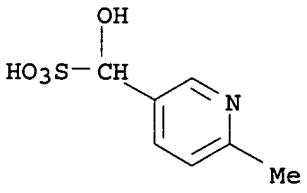
IT **283167-58-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone)

RN 283167-58-8 CAPLUS

CN 3-Pyridinemethanesulfonic acid, α-hydroxy-6-methyl-, monosodium salt (9CI) (CA INDEX NAME)



● Na

=>

```
=> s l2
L4            0 L2

=> fil biel
'BIEL' IS NOT A VALID FILE NAME
SESSION CONTINUES IN FILE 'CAOLD'
Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files
that are available.  If you have requested multiple files, you can
specify a corrected file name or you can enter "IGNORE" to continue
accessing the remaining file names entered.

=> fil bielstein
'BIELSTEIN' IS NOT A VALID FILE NAME
SESSION CONTINUES IN FILE 'CAOLD'
Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files
that are available.  If you have requested multiple files, you can
specify a corrected file name or you can enter "IGNORE" to continue
accessing the remaining file names entered.

=> fil beil
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.43     173.70

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                       0.00      -0.73

FILE 'BEILSTEIN' ENTERED AT 17:10:59 ON 10 NOV 2005
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FILE LAST UPDATED ON OCTOBER 10, 2005

FILE COVERS 1771 TO 2005.
*** FILE CONTAINS  9,363,954 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in
   separate documents and can not be searched together in one query.
   Reaction data for BEILSTEIN compounds may be displayed
   immediately with the display codes PRE (preparations) and REA
   (reactions).  A substance answer set retrieved after the search
   for a chemical name, a compounds with available reaction
   information by combining with PRE/FA, REA/FA or more generally
   with RX/FA. The BEILSTEIN Registry Number (BRN) is the link
   between a BEILSTEIN compound and belonging reactions. For mo
   detailed reaction searches BRNs can be searched as reaction
   partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE  <<<

**********************************************************************
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.                 *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE    *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE           *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                         *
* FOR PRICE INFORMATION SEE HELP COST                                 *
**********************************************************************
    NEW
* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE
  SEARCHED, SELECTED AND TRANSFERRED.
* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES,
  ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A
```

COMPOUND AT A GLANCE.

```
=> s l2
L5              0 L2
```